Problems in Pattern Formation, Geometry and Design of Materials

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Manipulating the micro-structure of material \(\rightarrow\) desired change in its mechanical responses.

- Actuation of thin nematic glass sheets
- Halftone gel lithography
- Understanding morphogenesis in response to inhomogeneous and incompatible prestrain
- Pattern formation: wrinkling / blistering / crumpling ...

Mathematical problems combining geometry, analysis, calculus of variations, pdes, related to practical questions of material design.

- Forward and inverse problems of isometric immersions
- Energy scaling laws
- Incompatible elasticity / dimension reduction
- Questions of regularity / uniqueness / existence of solutions to nonconvex problems
Geometric design problem in actuation of liquid crystals

Given: $S, \sigma_1, \sigma_2$
Find: $U, u$
so that:

$$\text{Spec}((\nabla u)^t \nabla u)(x) = \{\sigma_1(u(x)), \sigma_2(u(x))\}$$

1. Find eigenvectors $\hat{n}(x), \hat{n}^\perp(x)$ of $(\nabla u)^t \nabla u$
2. Align the liquid crystal director in the flat configuration with $\hat{n}(x)$
3. Spontaneous actuation of the metric $G$ will result in manufacturing surface $S$:

$$((\nabla u)^t \nabla u = (\sigma_1 \circ u)\hat{n} \otimes \hat{n} + (\sigma_2 \circ u)\hat{n}^\perp \otimes \hat{n}^\perp = G$$
Geometric design problem in actuation of liquid crystals

Among $y : U \rightarrow \mathbb{R}^3$ satisfying $(\nabla y)^t \nabla y = G$, the energy minimizing $y$ will be realised: $E(y) = \int_U |H_y|^2 \equiv \int_U |Iy|^2$

Another problem (more restrictive):
Given $g : S \rightarrow \mathbb{R}^{2 \times 2}_{sym, pos}$ prestrain metric on $S$
Find $u : U \rightarrow S$ such that $(\nabla u)^t \nabla u = g \circ u = G$

Energy minimization criterion as before. [Acharya-L-Pakzad’14]
Method of photopatterning polymer films that yields temperature-responsive gel sheets that can transform between a flat state and a prescribed 3d shape.

Lightly cross-linked dots embedded in a cross-linked matrix \( \rightarrow \) “nearly continuous” 2d “patterns of swelling” (prestrain metric \( G \))
Half-tone gel lithography

- **Forward problem:**
  Given $G$ on $U$, minimize: $E^h(y) = h^2 \int_U |I_2 y|^2 + \int_U |I y - G|^2$

- Euler-Lagrange equations given in terms of $I = I_y$ and $II = II_y$:

\[
F(I, II; G) = 0
\]

\[
(*) \quad \text{compatibility conditions via Gauss-Codazzi eqns boundary conditions}
\]

[Kim, Hanna, Byun, Santangelo, Hayward – Science, 2012]

- **Inverse design problem:** [Dias, Hanna, Santangelo – Phys. Rev. E, 2011]

Given $S$ with parametrisation $u : U \rightarrow S$, yielding: $I = I_u$, $II = II_u$

Solve $(*)$ for $G \Longrightarrow$ imprint $G \Longrightarrow$ activate for $S$
General set-up: Incompatible elasticity

\[ E(u) = \int_{\Omega} W(\nabla u \sqrt{G}^{-1}) \, dx, \quad u : \mathbb{R}^3 \supset \Omega \to \mathbb{R}^3 \]

- \( E(u) = 0 \) if and only if: \((\nabla u)^t \nabla u = G\) and \(\det \nabla u > 0\)
- \( \text{Riem}(G) \neq 0 \implies \inf_{u \in W^{1,2}(\Omega, \mathbb{R}^3)} E(u) > 0 \)

Dimension reduction for prestrained thin films:
\[ \Omega^h = U \times (-\frac{h}{2}, \frac{h}{2}), \quad E^h(u^h) = \frac{1}{h} \int_{\Omega^h} (\nabla u \sqrt{G}^{-1}), \quad G(x', x_3) = G(x') \]

Questions: 1. Scaling: \( \inf E^h \sim h^\beta \), 2. Asymptotics: \( \arg\min E^h \) as \( h \to 0 \)

Small energy theories \( \beta \geq 2 \implies \) only 2 residual theories!

**Theorem (L, Pakzad’09; Bhattacharya, L, Schaffner’14)**

\( \beta = 2 \). Only valid when: \( \exists y \in W^{2,2}(U, \mathbb{R}^3) \) \((\nabla y)^t \nabla y = G_{\text{tan}}\).
Then: \( \arg\min E^h \to \arg\min I_2(y) = \int_U |\text{sym}((\nabla y)^t \nabla b)|^2. \)

**Theorem (L, Raoult, Ricciotti’15)**

\( \beta = 4 \). Only valid when: \( R_{1212} = R_{1213} = R_{1223}(G) = 0 \).
\( \arg\min E^h \to \arg\min I_4 = \int_U |\text{stretching}|^2 + |\text{bending}|^2 + \int_U |\text{Riem}(G)|^2. \)
General set-up: Incompatible elasticity

- $\beta = 2$. Only valid when: $\exists y \in W^{2,2}(U, \mathbb{R}^3) \ (\nabla y)^t \nabla y = G_{\text{tan}}$.
  $I_2 = \int_U |\text{sym}((\nabla y)^t \nabla \tilde{b})|^2$.

- $\beta = 4$. Only valid when: $R_{1212} = R_{1213} = R_{1223}(G) = 0$.
  $I_4 = \int_U |\text{stretching}|^2 + |\text{bending}|^2 + \int_U |\text{Riem}(G)|^2$.

Questions:

- Uniqueness / multiplicity of minimizers to $I_2$
- Uniqueness / multiplicity of minimizers to the "linearized problem":
  $I_{2, \text{lin}}(v) = \int_U |\nabla^2 v|^2$; $\det \nabla^2 v = \text{curl}^t \text{curl} G_{\text{tan}}$
- Differences for positive / negative curvature of $G_{\text{tan}}$
- Geometry enters in a subtle manner; regularity questions for isometric immersions

[Klein, Efrati, Sharon - Science '07]
Wrinkling/ blistering/ crumpling ...

- In lower energy regimes, the minimizing sequences develop oscillatory behaviour $\Rightarrow$ energy relaxation
- Energy comparison methods $\Rightarrow$ certain patterns are energetically preferable

$$E^h(u^h) = \frac{1}{h} \int_{\Omega^h} W(\nabla u^h) + \left( \frac{T_{\text{in}}}{h} \int_{|x|=r} u \cdot \frac{x}{r} - \frac{T_{\text{out}}}{h} \int_{|x|=R} u \cdot \frac{x}{R} \right)$$

Then: $|\min_{u^h \in W^{1,2}} E^h - \min E_0| = O(h)$

where $E_0 = \text{relaxation obtained by quasi-convexification + boundary terms}$
Wrinkling/ blistering/ crumpling ...

- Example: Wrinkles of annular sheet loaded in the radial direction
  [Kohn, Bella – CPAM, 2014]

\[
E^h(u^h) = \frac{1}{h} \int_{\Omega^h} W(\nabla u^h)
+ \left( \frac{T_{in}}{h} \int_{|x|=r} u \cdot \frac{x}{r} - \frac{T_{out}}{h} \int_{|x|=T} u \cdot \frac{x}{R} \right)
\]

Then:
\[
\left| \min_{u^h \in W^{1,2}} E^h - \min E_0 \right| = O(h)
\]

where \( E_0 \) = relaxation obtained by quasi-convexification + boundary terms

- Lower bound estimates: \( \min E^h - \min E_0 \geq ch \)
- Upper bound construction of \( u^h \), informed by experimental ansatz
Wrinkling/ blistering/ crumpling ...

- Wrinkle to crumple transition
- Smooth cascades
- Other patterns

[King, Schroll, Davidovitch, Menon - PNAS’12]

[Huang, Davidovitch, Santangelo, Russell, Menon – PRL’10]

[Cerda, Mahadevan – PRL’03]

[Davidovitch et al., 2012]
Oscillatory behaviour $\implies$ lower regularity in the limit $\implies$ analytical difficulties (low regularity maps are “flexible”)

**Theorem (Nash, Kuiper – 1955. Convex integration for isom. immer.)**

Let $G$ be a $C^2$ metric. Then its $C^1$ isometric immersions are dense (w.r.t $C^0$ norm) in the set of all short immersions of $G$.

**Theorem (L-Pakzad – 2015. Convex integration for Monge-Ampère)**

Let $f$ be Hölder continuous. Then $C^{1,\alpha}$ solutions (for any $\alpha < \frac{1}{7}$) to $\det \nabla^2 v = f$ are dense in $C^0(U)$.

Thank you for your attention